

LA-UR-02-3258

*Approved for public release;
distribution is unlimited.*

Title: Progress in Statistical Crack Mechanics: An Approach to Initiation

Author(s): J.K. Dienes, T-14
J. Middleditch, CCS-3
J.D. Kershner, T-14
Q.H. Zuo, T-3
A. Starobin, T-14

Submitted to: 12th International Detonation Symposium
August 11-16, 2002
San Diego, CA



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Form 836 (8/00)

PROGRESS IN STATISTICAL CRACK MECHANICS: AN APPROACH TO INITIATION

J.K. Dienes, J. Middleditch, J.D. Kershner, Q.H. Zuo, A. Starobin

Los Alamos National Laboratory

Los Alamos, New Mexico, 87545

We have developed a general theory for the formation of hot spots from defects in explosives and propellants, and applied the theory to a variety of issues concerning the sensitivity of reactive materials. The defects of greatest concern in PBXs are cracks formed in the explosive grains, which are normally brittle. The theory accounts for the opening, shear, growth, and coalescence of cracks. In addition, the theory accounts for the heating caused by interfacial friction in closed (shear) cracks and the ignition process that results. Heat conduction and chemical reactions are treated on a smaller spatial scale than the overall continuum response; this is accomplished in the numerical (FEA) simulation with a sub-grid model. In previous work we have shown the feasibility of using this approach to model explosions that result from relatively mild insults, where many other hot-spot mechanisms fail. This paper addresses some of the complications that arise as mechanical failure and heating are examined in greater detail, including the effects of crack orientation, friction, melting, viscosity in molten regions, radial crack formation via a new approach to percolation theory, and 3-D effects.

INTRODUCTION

Crack formation in explosives is often observed, both macroscopically and in micrographs. This may occur as a result of initial formulation or subsequent damage. In SCRAM (Statistical CRACK Mechanics) we exploit the known behavior of cracks to characterize the initiation of explosives by impact at low speeds. Though open cracks are readily observed, in this application of SCRAM the underlying concept is that closed (shear) cracks, which are much less obvious, are responsible for initiation. When cracks

are closed we find that the heat generated by interfacial friction can cause a significant reaction. This mechanism allows for relatively large hot spots, and size is an important consideration in initiation, especially in seeking an explanation for the violent reactions observed in XDT, Steven, and HEVR tests¹. (Though the temperature can become high where grains rub together and at crack tips, the size of the high-temperature region is generally too small for formation of an explosive hot spot.) In the preceding symposium the SCRAM methodology was exploited by

Dienes and Kershner² to model the multiple-shock initiation of PBX 9501 reported by Mulford et al.³ with one-dimensional hydrodynamics. A multi-dimensional application to projectile impact was reported in the same symposium⁴, but those studies should be considered exploratory. One of the major challenges in analyzing hot spots is to determine which issues should be explored in greater detail. Five have been selected for this report.

Briefly, the five topics that have been receiving the greatest attention by us are the following: Orientation of the most unstable crack as a function of stress state, especially shear cracks with friction; Melting due to interfacial friction in shear cracks and subsequent viscous heating; Coalescence of micro-cracks into large (visible) mega-cracks; Improvements in modeling multiple-shock experiments with the HYDROX code; and Modeling three-dimensional impact behavior, especially radial cracks, with SCRAM in PRONTO.

CRACK ORIENTATION

In SCRAM we idealize the brittle behavior of real materials by treating the defects as an ensemble of randomly oriented, penny-shaped cracks that may be open or closed, stable or unstable, active or inactive, depending on the state of stress. The initial distribution of crack orientations is typically assumed to be isotropic (except for oil shale), but only a finite number of orientations is allowed, and we have usually taken the number we track to be nine. (We have run calculations with up to 490 orientations. In the ViscoSCRAM and IsoSCRAM approximations, crack orientation is not taken as a variable, and

only an average behavior is assumed.) Typically, some orientations are stable and others are unstable, resulting in anisotropic damage.

The question of crack stability as a function of orientation, accounting for the effect of interfacial friction in closed penny-shaped cracks, has recently been addressed by Zuo and Dienes⁵. (The importance of friction is illustrated by the fact that the compressive strength of brittle materials is typically about ten times the tensile strength, a fact we attribute to the effect of friction in resisting shear of compression cracks, while having no influence on tension cracks.) The goal of the analysis is to determine the most unstable crack orientation for all possible states of stress. It is shown that 5 types of brittle response are possible, whereas only 2 (opening and shear) are expected in the absence of friction. The types of behavior are tension (Mode I), combined tension and shear, pure (frictionless) shear (Modes II and III), shear with friction (splitting), and friction-locked. (Note that closed penny-shaped cracks experience both Mode II and Mode III behavior.) One unexpected result of the analysis is that the normal to the most unstable crack always lies in one of the principal-stress planes. As a result, the analysis and final results are taken to refer crack orientation to the principal axes of stress.

The five types of behavior are illustrated in Fig. 1, which assumes axial symmetry of the loading (triaxial stress) and divides a typical principal-stress plane into 9 sections. For this axisymmetric loading (which occurs in triaxial tests) σ_{11} denotes axial stress and $\sigma_{22} = \sigma_{33}$ denotes radial stress. For

sufficiently high stresses, axial and radial tension generate pure Mode I cracks (Type A); mixed opening and shear occur over a small range of loading angle (Type B); pure shear (no tangential traction) occurs for a range of loads that can be large if the coefficient of friction, μ , is large (Type C); "Splitting" occurs when the crack plane is nearly aligned with the greatest compression (Type D). A fifth type of response, in which the cracks do not influence the stress state, occurs when the interfacial friction exceeds the tangential component of traction (Type E). The range of stresses that can lead to reactive hot spots in explosives involves both compression and shear (Type D), as denoted by the darkest shading. Thus, four types of brittle response are unstable for sufficiently high stresses, (A, B, C, D), but a fifth type of response is

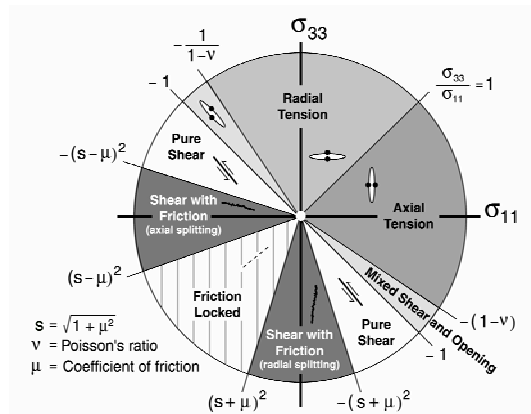


FIGURE 1. THE FIVE POSSIBLE TYPES OF BRITTLE BEHAVIOR AT HIGH STRESSES: MODE I CRACKING (TYPE A); MIXED OPENING AND SHEAR (TYPE B); PURE SHEAR (TYPE C); "SPLITTING," WHICH CAN LEAD TO REACTIVE HOT SPOTS (TYPE D); AND FRICTION-LOCKED (TYPE E).

possible in which all cracks are locked by interfacial friction (E).

One surprising result is that pure (frictionless) shear cracks occupy a significant fraction of the stress plane. This may explain one result of Howe, Gibbons, and Webber⁶, who examined damaged TNT in a 105mm round that was recovered, sectioned, and carefully polished following impact by a plate at 440m/s, as illustrated in Fig. 2. It is clear from a micrograph that there has been no significant reaction or friction on the long cracks at 45° to the impact direction. They can be considered as pure shear cracks (Type C). On the other hand, the shear-compression cracks (Type D) show clear evidence of reaction (blackening due to carbon). At an impact speed of 680m/s the shell explodes violently.

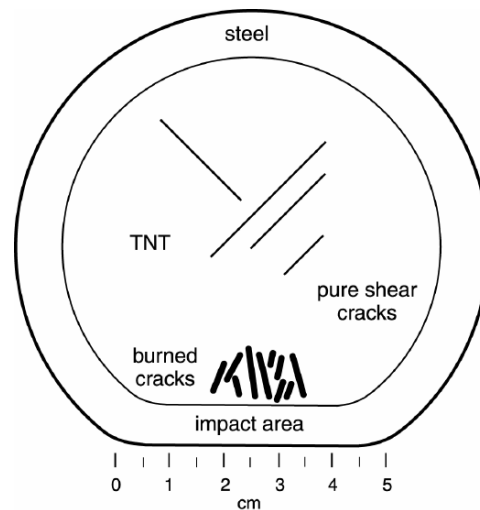


FIGURE 2. SKETCH OF PURE SHEAR AND SPLITTING CRACKS (TYPES C AND D) OBSERVED IN A 105 MM ROUND IMPACTED ON THE SIDE BY A FLYER PLATE AT 440 M/S (HOWE ET AL.⁶). A MICROGRAPH SHOWS NO EVIDENCE OF FRICTION ON THE PURE SHEAR CRACKS.

MELTING AND VISCOSITY

In the first analyses of cracking as an initiation mechanism, it was assumed that ignition could be modeled by solving the heat equation with an Arrhenius source term and a boundary condition representing the heat generation due to interfacial friction in closed penny-shaped cracks. The theory was successfully applied to explain XDT⁷, but as the theory was refined there was some concern that melting might play a role in reducing the heat generated when the crack surface reaches the melting point. On further analysis it appeared that the molten boundary layer at the crack surface is so thin that significant heat is produced by shearing of the viscous melt, especially when the crack is unstable⁷ but the latent heat of melting was accounted for only at the crack surface. More recently, we have refined the treatment of latent heat. To investigate its effect, we have developed a one-dimensional finite-difference ignition model containing an element between the molten and solid regions that accounts for discontinuous heat flux. Its motion accounts for the latent heat of melting. The algorithm has been validated in several ways. First, when the heat flux is held constant at the boundary the temperature rises according to the square root of time, as predicted by a well-known analytic solution. Second, the time to ignition with a fixed surface temperature, but no melting, is within a few percent of the time predicted using the theory of Linan and Williams⁸. Third, the energy balance accounting for heat input, viscous dissipation, reaction, and melting, is good to a few percent. Fourth, the results are insensitive to changes in resolution when $\Delta x^2 / \Delta t$ is

fixed. Fifth, a similarity solution has been found for the case when the temperature at a boundary is fixed (above the melting point) and a melt zone moves away from the boundary, with distance increasing with the square root of time, as shown in the appendix. The numerical and analytic solutions are compared in Fig. 3, showing agreement to within a few percent at a typical time. The precision could be increased by refining the numerics, but this does not seem justified at this point since few of the input data are known to better than a few percent accuracy, and they are not, in fact, constant. Furthermore, the assumption of one-dimensional heat flow due to friction in a penny-shaped crack is somewhat idealized.

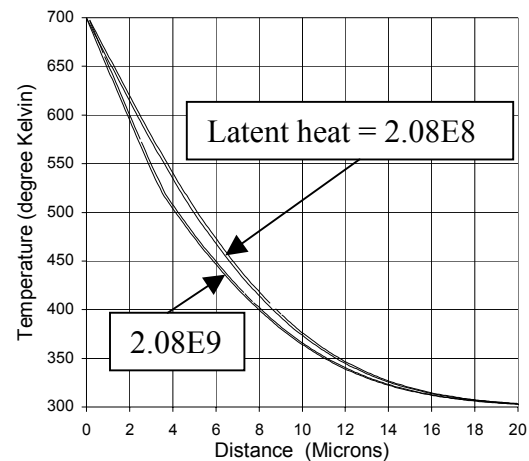


FIGURE 3. COMPARISON OF THE EFFECT OF LATENT HEAT ON THERMAL PROFILES ACCORDING TO ANALYTIC AND NUMERICAL SOLUTIONS. THE ANALYTIC SOLUTIONS LIE SLIGHTLY ABOVE THE NUMERICAL ONES.

In a typical initiation calculation the effect of latent heat was to increase the pre-ignition time 34%, from 139 to 187 μ s. This is the time when the Arrhenius

source term has contributed an amount of heat equal to 1% of the total heating. The actual latent heat was taken as 2.081×10^9 , while the lowered (and negligible) value was 2.081×10^8 . In that calculation the rate of heating was $1. \times 10^{11}$ ergs/cm²/s until the melting point (519K) was reached. After melting, viscous heating due to an assumed sliding velocity of 3500 cm/s produced a fairly intense source term because the molten layer was very thin ($7.94 \mu\text{m}$ at ignition for the estimated latent heat, $9.03 \mu\text{m}$ for the lowered value.)

A similar result may be obtained by considering the similarity solution of the appendix. In that case, when the surface temperature is fixed at 700K the melt layer moves $0.42 \mu\text{m}$ with latent heat accounted for, while it moves $0.53 \mu\text{m}$ (26% more) when the latent heat is reduced tenfold, as illustrated in Fig. 3.

The effect of viscosity is much more important. We considered two cases, the temperature-dependent viscosity of Bedrov, Smith, and Sewell⁹ and a constant value of 0.517 poise based on their data at a temperature of 650K. (Their fit is $3.46 \times 10^{-6} \cdot \exp(7744/T)$ in our cgs units.) Using the value of 0.517 poise, the ignition time is 2017 μs , while using the full temperature dependence the ignition time drops to 187 μs , the figure cited above.

The treatment appears to be flexible and sufficiently accurate. Thus, a second discontinuity representing the beta-delta transition can be implemented when sufficient data become available to represent the chemical-source term and the physical properties in the two phases separately.

COALESCENCE

The growth and coalescence of microcracks into networks can be observed in the formation of radial cracks near a point of impact¹, or during the cook-off experiments of Dickson et al¹⁰. Networks can form isotropically in principle, and this is the simplest case to model theoretically, but what is typically observed is the coalescence of nearly parallel cracks into large, nearly straight cracks. This behavior can be observed in the formation of spall fragments, but here we are concerned with the formation of cracks in the interior of explosives. The formation of networks has been addressed using percolation theory by chemists concerned with gels, physicists concerned with phase changes, and numerous others. Here we are concerned with crack behavior, which is conceptually similar but quite different in detail.

A crack in a random, homogeneous, isotropic ensemble of cracks has a certain probability of intersecting another crack denoted by p . It is assumed by Dienes¹¹ that cracks can no longer grow after a certain number of intersections that we denote by α , a number between 3 and 4. The average number of cracks that have intersected to form a connected set has recently been derived by Dienes¹², and is given by $\bar{n} = 1/(1 - \alpha p)$. As the cracks grow, p increases from nearly zero to $1/\alpha$, when the number of connected cracks becomes infinite and the material can be considered fully comminuted. These microcracks (typically under a hundred microns in diameter) may be open or closed.

The formation of plane macroscopic (centimeter) cracks is analogous, except in that case the only relevant cracks are those nearly in the plane of the large linear crack (megacrack) being formed. Only tensile cracks are considered in the formation of megacracks, since we are concerned primarily with the formation of radial cracks by tensile hoop stresses and in spall. The formation of radial cracks requires that the distribution of crack sizes vary randomly, since otherwise tension cracks would form uniformly in all the cells around the impact area. Thus, a SCRAM subroutine has been formulated that varies the initial crack radii following the exponential law that we have assumed elsewhere.

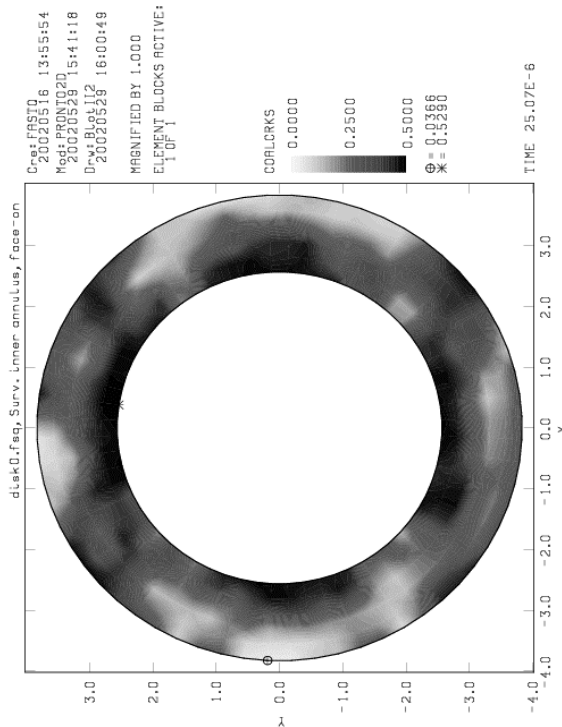


FIGURE 4. ILLUSTRATION OF THE FORMATION OF MEGACRACKS BY COALESCENCE OF MICROCRACKS WITH RANDOM INITIAL RADII IN AN INITIALLY SYMMETRIC RING.

Results of a test calculation are shown in Fig. 4, which illustrates the two new features of SCRAM: a random choice of crack radii and coalescence of microcracks into megacracks. The ring is not intended to simulate any real situation, but is serving as a diagnostic tool in validation. The shading represents the radii of megacracks formed where the tension exceeds a critical value.

MULTIPLE-SHOCK RESPONSE

A two-material flyer plate impacts an HMX target in the experiment of Mulford et al.³, resulting in two shocks, but only the second one is followed by significant reaction. In the Eleventh Symposium it was shown² that this experiment can be modeled with SCRAM, the reacting cracks beginning to burn shortly after the second shock as a result of interfacial friction and heating. In more recent work, the treatment of the burning cracks has been represented in greater detail using crack opening and radius as the two generalized coordinates in a pressurized-crack model using Lagrange's equations¹³. A subsequent paper¹⁴ showed that individual cracks are stable because crack growth is so fast (roughly sound speed) that the internal pressure drops rapidly, quenching the burn. However, it was found that large fluctuations in pressure caused by crack interactions could lead to highly unstable behavior of an ensemble of cracks. We hypothesize that this kind of behavior is responsible for the observed reactions.

More recently, we have been accounting for the late-stage behavior of the burned HMX by introducing a mixture rule into SCRAM. This allows

the solid to be represented by a Mie-Gruneisen equation of state while the burn products are characterized by a polytropic gas law, using the burning crack model cited above. Results are illustrated in Fig. 5. The late-time behavior is improved over previous calculations, but a better theory for the behavior of the burned gases under high pressure is clearly needed.

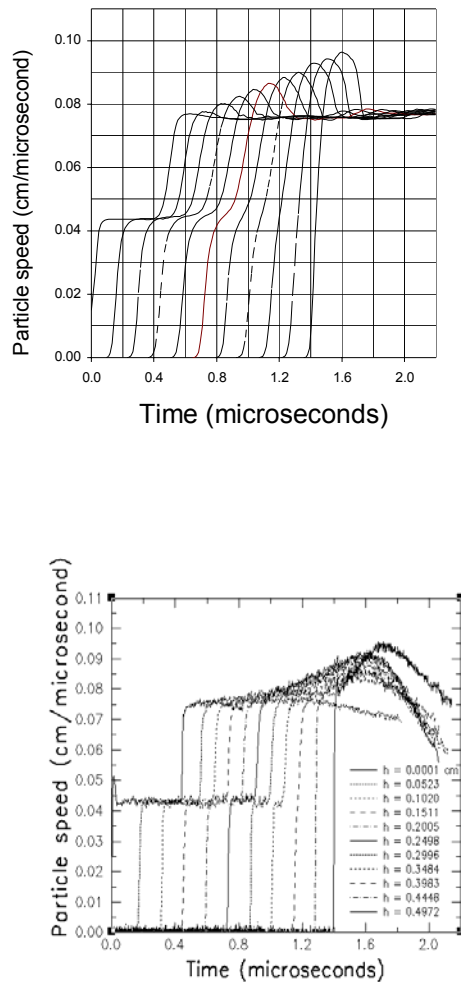


FIGURE 5. SCRAM-HYDROX CALCULATION OF MULTIPLE-SHOCK EXPERIMENT (ABOVE) COMPARED WITH THE MEASUREMENTS OF MULFORD ET AL.³ (BELOW).

SPRINTO

The basic SCRAM model can be incorporated into the three-dimensional version of PRONTO with no essential change, though it is important to vectorize the code to achieve reasonable computing times. An important three-dimensional effect that we can capture with this new code is the effect of radial cracks. Since the number of radial cracks is typically about five, the behavior is far from axisymmetric. To model such behavior we need to introduce a random distribution of cracks sizes, else all directions would behave in the same way. This is conceptually straightforward, since we are already assuming a random (exponential) distribution of crack sizes-it is merely necessary to add a random number generator that produces varying crack sizes in the initializing subroutine. Still, this does not allow for the coalescence that can be observed in the formation of large cracks. This has been addressed by the new coalescence theory described above.

CONCLUSIONS

As we examine in greater detail the influence on initiation of microcrack growth, coalescence, heating, and melting, the evidence for their importance increases, but this work is still considered a feasibility study to ascertain whether brittle failure can explain the violent reactions observed following mild damage¹⁻⁴. Recent work⁵ shows the sensitivity of crack behavior to friction and orientation, suggesting that far more than 9 orientations are needed to capture crucial crack behavior. Additional work is needed to account for

the role of phase changes in the later stages of ignition, as well as more accurate treatments of heat diffusion and chemical kinetics. The late stages of burn require a more detailed treatment of the burn algorithm and the equation of state. Crack interactions appear to play an important role, thus explaining the heterogeneous behavior observed in wave fronts and discussed by W. Davis¹⁵.

ACKNOWLEDGEMENTS

This work was performed with the financial support of the ASCI and MoU programs at Los Alamos.

REFERENCES

1. Idar, D.J., Lucht, R.A., Straight, J.W., Scammon, R.J., Browning, R.V., Middleditch, J., Dienes, J.K., Skidmore, C.B., and Buntain, G.A., "Low Amplitude Insult Project: PBX 9501 High Explosive Violent Reaction Experiments," in Eleventh Detonation Symposium, Snowmass, CO, J.M. Short and J.E. Kennedy, Chairmen, Aug. 31-Sept. 4, 1998.
2. Dienes, J.K. and Kershner, J.D., "Multiple-Shock Initiation via Statistical Crack Mechanics," Proceedings of the Eleventh International Detonation Symposium, Snow-mass, CO, Aug.30-Sept. 4, 1998, pp. 717-724.
3. Mulford, R.N., Sheffield, S.A., and Alcon, R.A., "Initiation of Preshocked High Explosives PBX 9404, PBX 9502, PBX 9501, Monitored with In-Material Magnetic Gauging," Proceedings of the Tenth International Detonation Symposium, Boston, MA, July 12-16, 1993, pp. 459-467.
4. Scammon, R.J., Browning, R.V., Middleditch, J., Dienes, J.K., Haberman, K.S., Bennett, J.G., "Low Amplitude Insult Project," Proceedings of the Eleventh International Detonation Symposium, Snowmass, CO, Aug.30-Sept. 4,1998, pp. 111-118.
5. Zuo, Q.H. and Dienes, J.K., "On the Types of Brittle Failure," in preparation.
6. Howe, P.M., Gibbons, G.G., and Webber, P.E., "An Experimental Investigation of the Role of Shearing Initiation of Detonation," Proceedings of the Eighth Symposium on Detonation, Albuquerque, NM, July 15-19, 1985, pp. 294-306.
7. Dienes, J.K., "A Unified Theory of Flow, Hot Spots, and Fragmentation with an Application to Explosive Sensitivity," in High-Pressure Shock Compression of Solids II, Springer-Verlag New York, Inc., Lee Davison et al., eds., 1996, pp. 366-398.
8. Linan, A. and Williams, F.A. "Theory of Ignition of a Reactive Solid by Constant Energy Flux," Combustion Science and Technology, **2**, 1970, pp. 11-20.
9. Bedrov, D., Smith, G.D., and Sewell, T.D., "Temperature dependent shear viscosity coefficients of HMX, a molecular dynamics simulation study," J. Chem. Phys., **112**, 2000, pp. 7203-7208.
10. Dickson, P.M., Asay, B.W., Henson, B.F. and Fugard, C.S., "Observation of the Behavior of Confined PBX 9501 Following a Simulated Cookoff

Ignition,” Proceedings of the Eleventh Detonation Symposium, Snowmass, CO, J.M. Short and J.E. Kennedy, Chairmen, Aug. 31-Sept. 4, 1998, pp. 606-611.

11. Dienes, J.K., “A Statistical Theory of Fragmentation Processes,” *Mech. of Materials*, **4**, 1985, pp. 325-335.

12. Dienes, J.K., "A Coalescence Algorithm for Radial and Spall Cracks," In Progress Report for FY 2001, The Joint DoD/DOE Munitions Technology Development Program, Los Alamos National Laboratory Report, in preparation.

13. Dienes, J.K., “Crack dynamics via Lagrange’s equations and generalized coordinates,” *Acta Mechanica*, **148**, 2001, pp. 79-92.

14. Dienes, J.K. and Kershner, J.D., “Crack dynamics and explosive burn via generalized coordinates,” *Journal of Computer-Aided Materials Design*, **7**, 2001, pp. 217-237.

15. Davis, W., Private communication, 2002.

APPENDIX

This appendix considers the role of latent heat in the thermal response of shear cracks by developing an analytic solution to the conduction problem. This allows us to validate the numerical procedure used in the more general initiation problem. The usual heat equation $\rho C_v \dot{T} = k T_{xx}$ with fixed temperature at $x=0$ and a moving melt front has a similarity solution of the form $T = f(\eta)$, $\eta \equiv x/\sqrt{4Dt}$. As usual,

$D \equiv k/\rho C_v$ is taken as the diffusion constant. At $x=0$ the temperature is taken as T_s , and at the melt front $T = T_m$. The effect of latent heat, L , is accounted for by the boundary condition $\rho L v = k \Delta T_x$ at the moving melt front, with v the velocity of the melt front and ΔT_x the discontinuity in the temperature gradient. A similarity solution of the form $f = C_1 \text{erf}(\eta) + C_2$ is valid on both sides of the melt front. It can be readily verified that the boundary condition at the melt front is consistent with a front speed of $v = \alpha/\sqrt{4Dt}$ and the similarity variable there is denoted by $\eta = \eta_0$. The boundary condition then reduces to

$$\frac{q-1}{\text{erf}(\eta_0)} - \frac{1}{1-\text{erf}(\eta_0)} = \alpha \eta_0 e^{\eta_0^2},$$

where $q \equiv T_s/T_m$, $\alpha \equiv 2L/C_v T_m$. This transcendental equation for η_0 has to be solved numerically, but the techniques are well known. The numerical procedure for integrating the heat equation with the boundary conditions for this similarity solution compares with the analytic solution to within a few percent in the thermal gradient at the boundary ($x=0$), the two gradients at the melt front, and in melt speed. Comparison of temperature profiles is illustrated in Fig. 3.